EGUSPHERE-2025-107 Author's comment to RC2 by Anonymous Referee #1 (Miriam Latsch et al.)

<u>Legend</u>: Referee comments in **black**, author comments in **blue**, changes in the manuscript text in **green**

The manuscript presents a worldmap of patterns of enhanced NO2 over oceans that can be attributed to ship tracks or oil rigs, based on high-pass filtered NO2 measurements from TROPOMI. The paper is well generally well written, and the resulting ship tracks are impressive by the presented detail.

We want to thank Referee #1 for the feedback and helpful comments on our manuscript. Detailed responses to the reviewer's comments can be found below. We hope that we have incorporated all suggestions and comments in a satisfactory way. At the end of this document, you will find a general section on additional changes we made during the review process.

I have the following general concerns:

- The paper presents patterns in a rather qualitative way (tSCDs), while in the title as well as in some instances in the text it sounds as if the study aims to quantify ship emissions. This should be avoided.

We agree with this comment and in response the title has been changed (see below). In addition, we have changed the term "NOx emissions" to "NO₂ signals" in Lines 419, 460, and 481. Furthermore, we have added the term "qualitative" or "qualitatively" to Lines 5, 55, 419, 460, and 481.

- The methodology should be clarified and the individual retrieval/filtering steps should be illustrated for real measurements.

Done; see below for details.

- The comparison to CAMS VCDs is problematic, as this dataset has not been high-pass filtered. This should be modified, or discussed properly.

Thank you for this hint. We discussed this in detail below.

- The outlook/next steps should be discussed in more depth. Obviously, it would be desirable to quantify NOx emissions for the detected ship tracks. How to do this, which problems have to be solved? (impact on filter settings, AMFs, ...)

Thank you for this comment. We have added the following sentence to Line 485:

"The next step for quantitative estimation of NOx emissions for the detected shipping tracks is, for example, to calculate the vertical columns using pixel-specific AMFs, including the dependence on observation geometry, surface reflectance, clouds and a priori NO₂ vertical profile."

Detailed comments:

Title: The title is misleading, as it suggests that this study is about quantifying ship emissions. Please consider modifying this, especially in the manuscript, for instance in line 149: I would expect to read a number at the end of the section with such a headline.

Thank you for pointing this out. We agree with you. The title of our manuscript has been updated to: "Improved detection of global NO₂ signals from shipping in Sentinel-5P TROPOMI data"

The headline of Section 3 has been changed to:
"3 Global shipping signals in filtered TROPOMI NO₂ tSCDs"

A statement like that in line 382 should already be made in the abstract.

"qualitatively" has been added to the sentence in Line 5 of the Abstract.

Line 4, line 49: This TROPOMI pixel size only holds for nadir. Towards the swath edges, pixels are considerably larger.

Thank you for this clarification. We added "at nadir" to the sentences in Lines 4 and 49.

Line 90: I agree that the tSCD allows the detection of ship NOx without bias from a-priori knowledge used for the AKs in the operational product. However, as soon as NOx emissions should be quantified, the tSCDs need to be converted to tVCDs by an (appropriate) AMF.

Thank you very much for pointing that out. You are right that an appropriate and pixel-specific AMF is needed to convert the tSCDs into the tVCDs for the quantification of ship emissions. In this study, we only want to qualitatively detect the shipping signals in the TROPOMI data. Therefore, we used the tSCDs to avoid any influences of model-based parameters on the measurements obtained from the operational TROPOMI product. We feel that it is important to first establish that the signals in the satellite data are genuine and then use a priori data (not necessarily from models) where needed.

Please clarify.

Lines 93-104: I think a short modification sentence would be helpful: The tSCD is provided in the operational product (or could easily be calculated by subtracting V_strat*AMF_strat from total SCD), but this quantity turned out to be affected by a simplification in the operational processor: ...

Thank you for this hint. We implemented your suggestion to the sentence in Line 93: "The tSCD is provided in the operational product, but this quantity turned out to be affected by a simplification in the operational processor, as distinct box-like patterns were noticed in the TROPOMI NO₂ data during data processing."

Line 106: What does "approximately" mean?

We use 33 pixels with a resolution of 0.03° for the standard high-pass filter, so the resulting box size is 0.99° (approximately 1°). We thought it might be more helpful for readers to know the degree value rather than the number of pixels used, as it is easier to visualize and more consistent. These numbers (33 pixels for the 1° box size and 9 pixels for the 0.25° box size) are also mentioned in Appendix A1, which explains the high-pass filtering in more detail.

Line 109: How far is this a "saturation"? What is saturated?

The "saturation" of the high-pass filtered tSCDs refers to the saturation of the color scale by values up to 1e14 molec cm⁻² large. The occurrence of these very high values depends on the region. An example of only high-pass filtered data is shown in Fig. B2. The values greater than 3e13 molec cm⁻² corresponding to this saturation occur mainly in the south and southeast of the coastline in the Arabian Sea and the Gulf of Oman. We have changed the sentence in Line 109 to:

"However, due to taking the rolling mean on the data, the high-pass filtered tSCDs show a saturation of the color scale by very high NO₂ values at some coastlines and negative values around the highlighted shipping lanes."

Filtering: The iterative filter approach seems complex, and Fig. 1 does not really help. I would propose to have a sketch showing the effect of the individual steps on real data instead.

Thank you for this suggestion. We have added illustrations of the various variables resulting from the different filtering steps to the variable names in Figure 1 and updated its caption.

Fig. 2 shows the result of the iterative filter process. I do not understand how the values here can exceed 4e13, when in a previous step everything above 3e13 has been skipped. Please clarify.

The threshold value of 3e13 was only used in Step 2 to mask the highest and lowest values of the high-pass filtered data that localize the shipping routes. After applying this mask to the gridded data in Step 3, the gridded values are interpolated again in Step 4. Therefore, after the following high-pass filtering step with these interpolated values, corresponding values higher than 3e13 reappear in Step 5. This iterative method highlights the shipping lanes more accurately with each repetition. We hope these processing steps are now easier to understand by adding the real data illustrations to Figure 1, as you suggested above.

Line 149: Even with stating the disadvantages of applying filters, one might think that all the discussed filters are applied below. A statement should be added that, as default, they are *not*, with reference to later discussion why not.

We explained in Line 152: "As the standard criterion, no data flagging is applied to the filtered TROPOMI NO₂ tSCDs, as discussed later.". However, we have added the following sentence in Line 149 to clarify this beforehand:

"Sect. 3.1 discusses the individual impacts of the various flagging criteria in detail, while no flagging criterion is applied to the tSCDs as a standard in this study."

Line 157: except the model used for assimilating strat. NO2...

That's right! We added "tropospheric" to the sentence.

Fig. 3: The map of resulting ship tracks is quite impressive, and the benefit of 1° over 0.25° quite prominent. However, this is a result of the high-pass filter, and this will inevitably cause *negative* tSCDs next to the shipping lines. This would have to be taken into account for quantification of emissions. I thus think that the figures should also show the negative values to create awareness for this effect - this might not look as nice, but more honest.

You have made a point. Although the negative values are already represented in the cross-sections, we agree that more awareness should be created for them. Therefore, we added a figure to the Appendix, which shows a global map with a symmetrical color scale. In addition, we added the following paragraph in Line 149:

"Another essential aspect to consider is that the choice of the maps' color scale significantly affects the visualization of the shipping lanes. When a symmetric color range with equally distributed negative and positive limits is used, the negative values in some coastal regions become more prominent on the map (see Fig. B1). In contrast, shifting the values to a positive color range highlights the shipping lanes more effectively (see Fig. 2). This study focuses on the qualitative detection of shipping signals. Therefore, a positive color scale is used for the maps."

Furthermore, the following sentence has been added to the caption of Figure 2: "Fig. B1 shows the corresponding global map of the filtered TROPOMI NO₂ tSCDs using a symmetric color scale to visualize also the negative values resulting from the high-pass filtering method, which occur mainly at coastlines around Europe and Asia." The reference to this Appendix figure has been added to Line 269, where the negative values are also explained in the cross-sections.

CAMS comparison:

Are the CAMS tVCDs high-pass filtered as well? If not, they should for a more meaningful comparison.

Good point; thank you very much for this hint! In the preprint document, only an offset was removed from the CAMS data. We now high-pass filtered the CAMS model data with the same high-pass filtering settings, adding this information in Line 386:

"To ensure a consistent analysis, the CAMS model data are high-pass filtered with the same settings as the TROPOMI data with a tenfold iteration. Consequently, 3 pixels of the CAMS model data are used for the rolling mean applied to the high-pass filter to maintain the 1° box size."

We have changed Figures 11, C1, C2, and C3 and their captions and updated Section 4, the Abstract (Lines 15-18), and the Conclusions section (Lines 468-480) with the modified results and the term "high-pass filtered CAMS data" or the like. In addition, we added a second figure for the South Atlantic shipping lane (Fig. C4), using a decreased threshold for the masking in the high-pass filtering method since we found a large dependence of the CAMS model data on this defined threshold value in this region. We added the following paragraph to Line 418 to discuss this issue:

"For the shipping route in the South Atlantic (Fig. C3c), the peak of the CAMS curve is twice as large as those of the TROPOMI curves, which do not exceed 0.5e13 molec cm⁻². It appears to be slightly shifted due to the lower number of values resulting from the coarser spatial resolution. The difference between the two data sets is small with these standard settings. However, Fig. C4 shows that the high-pass filtered CAMS NO2 data for this shipping lane strongly depends on the masking threshold used in Step 2 of the high-pass filtering method (see Sect. 2). When the masking threshold value is lowered to ±1e13 molec cm⁻², the high-pass filtered CAMS NO₂ tVCDs increase extraordinarily and are at least three times higher than with the standard threshold of ±3e13 molec cm⁻² (Fig. C3). The higher peak is accompanied by a much broader FWHM, so the shipping lane expands over the entire polygon area. This large dependence on the choice of masking threshold is only found for the shipping lane in the South Atlantic and only for the CAMS NO2 data when considering the three selected regions. In contrast, the TROPOMI data show slightly higher peaks, where the difference is consistent and comparable to the other shipping lanes. Therefore, it should be kept in mind that applying the high-pass filter to the CAMS model data may result in large changes of the values in some regions, depending on the threshold value chosen."

Line 421: and avoiding artificial ship tracks just introduced by the a-priori profiles?

Thank you. Your suggestion has been added to the sentence:

"By focusing on NO₂ tSCD rather than tVCD, a more objective identification of NO_x emissions from shipping is obtained, benefiting from the enhanced spatial resolution and avoiding artificial ship tracks introduced by the a priori profiles, associated with limitations of the AMFs derived from the coarse TM5 model, which only inadequately captures localized emissions."

Fig. C1: This comparison is not appropriate, since the TROPOMI data has been high-pass filtered, but the CAMS data not. At least this aspect needs to be clearly discussed.

Thank you for your comment. We have already discussed this point and the changes applied above. All CAMS model data are now also high-pass filtered.

A statement on data availability is missing. I would encourage the authors to make their results available on a data repository so that future studies could reference this dataset with a doi.

The data set has been submitted to the PANGAEA repository, has been reviewed and can be published as soon as the paper manuscript is published. The DOI of the data set has already been implemented in the manuscript but has not yet been registered. The data set can be accessed via the following temporary link:

https://www.pangaea.de/tok/e6a3d2eb22f88dc8930d73b32e3775384d6c3642. The paragraph on data availability has been updated to:

"The data sets of the global filtered TROPOMI NO₂ tSCDs for different box sizes of the high-pass filter (1°, 0.5°, 0.25°) and for the standard box size of 1° with the various flagging criteria, as displayed for example in Fig. 2, are freely available from PANGAEA (Felden et al., 2023) under the CC-BY-SA license (Latsch et al. (2025), https://doi.org/10.1594/PANGAEA.982514)."

Other changes made to the manuscript during the review process:

All figures with maps (Figures 2-7, 9-11, B1-B2, and C1-C3) have been changed: The inland water pixels are now also flagged as NaN values to focus on the ocean regions and to reduce the scatter over the continents.

Additionally, Figure B1 and Figure C1: The surface classification mask of the TROPOMI data is now also applied to the CAMS data. Thus, the same pixels are flagged as NaNs for visual consistency. The reason why these water pixels are marked as invalid is that the TROPOMI surface classification mask defines snow and ice pixels over water as land pixels. In this study, only water pixels are included. However, these flagged pixels are irrelevant for this study because they represent the snow and ice edge and, therefore, are not affected by ship emissions.

We added the following sentence to the Acknowledgments:

"We thank the two anonymous reviewers for their comments and suggestions which helped to improve the results and their presentation in this manuscript."